

Surface states and the thermal Casimir interaction

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Abstract – Using exact calculations, we elucidate the significance of the surface (bound) states for the thermal Casimir interactions for an Ising strip with a finite width. The surface state arises whenever an imaginary wavenumber mode appears in the spectrum of the transfer matrix, taken in the direction parallel to the edges of the strip. Depending on the boundary conditions, the imaginary modes emerge below or above the bulk critical temperature, or below the wetting temperature of a single surface with surface magnetic field. The bound states are responsible for the strong asymmetry of the Casimir forces between the super- and sub-critical regimes and for their sign. Our analysis uses the fact that the Casimir forces have two mathematical forms. We show that these very different representation are the same and in the process find the origin of the asymmetry.

It has been known for about half a century that the existence of quantum fluctuations in the electromagnetic vacuum is revealed by the existence of long-ranged, largely attractive, forces between objects [1]. For instance, in the geometry of parallel plates at a distance L apart, the wavenumbers in the direction perpendicular to the plates become discrete and this produces a change in the energy, which (per unit area) behaves as $\delta E(L) \propto \hbar c/L^3$ for sufficiently large distances, c is the speed of the light and \hbar is a Planck's constant. Fisher and de Gennes [2] made the crucial observation that in condensed matter systems, say uniaxial classical ferromagnets and their analogues, the confining surfaces restrict order parameter fluctuations leading to to "entropic" forces between the surfaces. Scaling theory applied to these fluctuations predicts the existence of forces per unit area in the critical region (at zero bulk field) of the form (in the following all free energies and forces are expressed in units of $k_B T$)

$$\mathcal{F}_{Cas} = L^{-d} \Theta(\text{sgn}(T - T_c)L/\xi) \quad (1)$$

where T_c is the bulk critical temperature, ξ is the bulk correlation length and the distance between the confining surfaces is L [2]. These forces are of significance on the micro- and nanoscale as shown in experiments on wetting

films and colloidal systems [3–6].

The finite-size scaling function Θ is expected to depend on the geometry and on the boundary conditions (BCs) imposed by the confining surfaces. Mathematical consistency may allow small and large argument behavior in (1) to be inferred, but to go further, detailed calculations of Θ are needed. The main generally applicable techniques are Monte-Carlo simulations [7] and the de Gennes-Fisher-Upton local functional method [8]. The success of the first depends crucially on a thorough understanding of finite-size effects; the second is phenomenological in character, but with the benefit of containing no adjustable parameters. In view of these matters, exactly solvable models have a special relevance, since they afford insights not otherwise available.

In this Letter, we shall consider Casimir forces in the planar Ising model with a strip geometry. This encompasses binary mixtures and lattice gases, with the surface magnetic fields playing the role of surface (differential) fugacities. Depending on the method of calculation used to obtain them, the results of the Casimir force come in two very different *mathematical* forms. One of them, a *mode sum*, has received little analytical attention so far. It has two advantages: firstly, the finite geometry imposes the

discretisation condition in this mode sum, as in the quantum Casimir case. The second advantage, and this is one of the results of this Letter, is that the strong asymmetry between the super- and sub-critical regimes receives for the first time a *microscopic* interpretation through the contribution of bound states, or surface modes. Their existence in this context has been known for quite some time [9], but not the interpretation, which we provide in this Letter in terms of the Fisher-Privman finite-size scaling theory [12]. The other representation of the Casimir force for strips, this time as an *integral*, comes either from Au Yang and Fisher [13, 14] or from extension of the Schultz, Mattis and Lieb (SML) method [15, 16], with the following advantages: it is ideal for taking the scaling limit, and also for investigating real analyticity in x of $\Theta(x)$ from (2). Further, although it is the obvious choice for numerical work, it gives no insight into the striking asymmetry mentioned above [17]. The most recent contribution along this line explains how the boundary fields can be adjusted to produce both attractive and repulsive critical Casimir interactions [17].

We now specify the model more precisely. As shown in Fig. 1, we have an Ising strip with cyclic BCs in the $(1, 0)$ direction. The energy for a configuration $\{\sigma\}$ of spins is

$$E_{N,M}(\{\sigma\}) = - \sum_{m=1}^M \sum_{n=1}^N K_1 \sigma_{m,n} \sigma_{m+1,n} \quad (2)$$

$$- \sum_{m=1}^M \sum_{n=1}^{N-1} K_2 \sigma_{m,n} \sigma_{m,n+1} + E_{\text{boundary}}.$$

The term E_{boundary} just concerns the rows $n = 1$ and $n = N$. This situation can be handled by a transfer matrix (TM) building the lattice in the $(0, 1)$ direction, where the matrix has cyclic symmetry in the $(1, 0)$ direction; the SML technique [15] may be applied. The alternative is to transfer in the $(1, 0)$ direction; cyclic symmetry no longer obtains, but the TM spectrum can still be found [9, 18–20] for the BCs which we consider.

The free energy per unit length in the $(1, 0)$ direction, as derived from the transfer in the $(0, 1)$ direction is [17]

$$f(N) = -\frac{1}{4\pi} \int_{-\pi}^{\pi} d\omega \ln \left[A_1 A_2 e^{N\hat{\gamma}(\omega)} + B_1 B_2 e^{-N\hat{\gamma}(\omega)} \right] \quad (3)$$

up to an additional term $(N/2) \ln(\sinh 2K_2)$. Here, $\hat{\gamma}(\omega)$ is the Onsager function given by [21]

$$\cosh \hat{\gamma} = \cosh 2K_1 \cosh 2K_2^* - \sinh 2K_1 \sinh 2K_2^* \cos \omega, \quad (4)$$

where the non-negative real branch is taken for real ω , K_j^* is the dual coupling given by the involution $\sinh 2K_j \sinh 2K_j^* = 1$, $j = 1, 2$; $A_j(\omega)$ and $B_j(\omega)$ depend on the BCs. For free boundaries, we have $A_1 = A_2 = e^{\hat{\gamma}} \cos(\hat{\delta}'/2)$ and $B_1 = B_2 = e^{-\hat{\gamma}} \sin(\hat{\delta}'/2)$, for $(+, +)$ BCs with all spins on the bottom and top boundary fixed

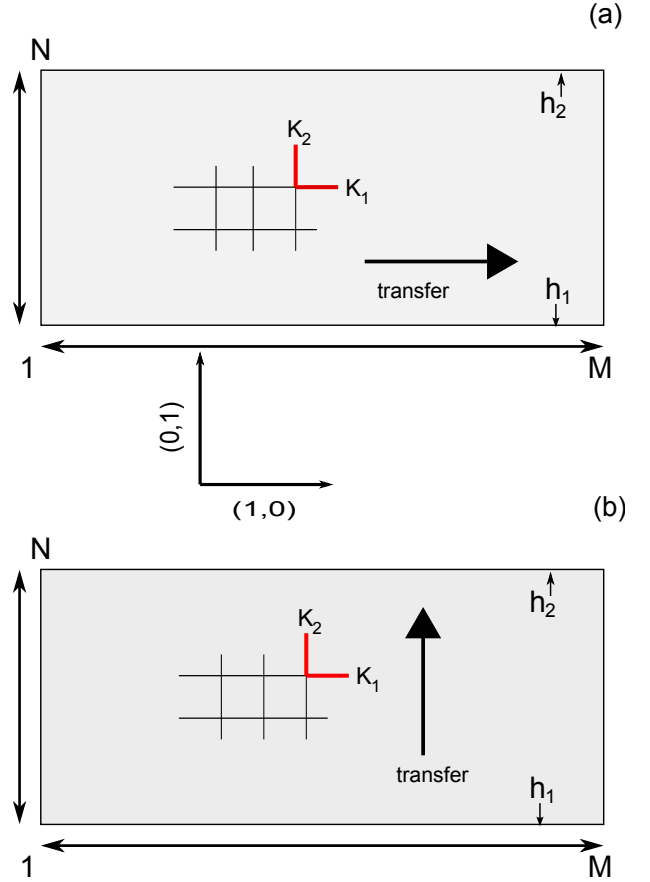


Fig. 1: (color online) An Ising strip with M columns and N rows. We are interested in the limit $M \rightarrow \infty$ with $N < \infty$. Surface fields h_1 and h_2 are applied at the bottom and top edges; in the present paper we consider free boundaries $h_1 = h_2 = 0$ and the $(+, +)$ boundary conditions $h_1 = h_2 = \infty$. In the model (a) the transfer matrix is along the $(1, 0)$ axis whereas in the model (b) along the $(0, 1)$ direction.

at the value $+1$, we have $A_1 = A_2 = e^{\hat{\gamma}} \cos(\hat{\delta}^*/2)$ and $B_1 = B_2 = e^{-\hat{\gamma}} \sin(\hat{\delta}^*/2)$. The angles $\hat{\delta}^*$ and $\hat{\delta}'$ are elements of the Onsager hyperbolic triangle [21], given by the formula $\sin \hat{\delta}'(\omega) = \sinh 2K_1 \sin(\omega) / \sinh \hat{\gamma}(\omega)$ and $\cos \hat{\delta}' = (\cosh 2K_2^* \cosh \hat{\gamma} - \cosh 2K_1) / (\sinh 2K_2^* \sinh \hat{\gamma})$. The angle $\hat{\delta}^*(\omega)$ has K_1^* and K_2 interchanged. Extracting from (3) the bulk contribution $Nf_\infty = -N(1/4\pi) \int_0^{2\pi} \hat{\gamma}(\omega) d\omega$, which is easy, and an additional, N independent, surface contribution $f_s = -(1/4\pi) \int_0^{2\pi} \log [A_1 A_2] d\omega$ gives the Casimir free energy:

$$\mathcal{F}_{Cas} = -\frac{1}{4\pi} \int_{-\pi}^{\pi} d\omega \ln \left(1 + e^{-2N\hat{\gamma}(\omega)} \tan^2 \left(\hat{\delta}(\omega)/2 \right) \right), \quad (5)$$

where $\hat{\delta}(\omega) = \hat{\delta}_1(\omega) + \hat{\delta}_2(\omega)$, and $\hat{\delta}_i(\omega)$, $i = 1, 2$ depend on the BCs. For free boundaries $\hat{\delta}(\omega) = \hat{\delta}^*(\omega)$, whereas for $(+, +)$ BCs $\hat{\delta}(\omega) = \hat{\delta}'(\omega)$.

On the other hand, the transfer matrix V for the $(1, 0)$ direction has the diagonal form [9, 18–20]

$V = \exp \left[-\frac{1}{2} \sum_{j=1}^N \gamma(\omega_j(N)) (2X_j^\dagger X_j - 1) \right]$. The X_j are Fermion operators with anticommutation relations: $[X_j, X_l]_+ = 0$, $[X_j, X_l^\dagger]_+ = \delta_{jl}$. Thus $2X_j^\dagger X_j - 1$ has eigenvalues ± 1 . They are a linear combinations of the spinor operators Γ_n [15]:

$$X^\dagger(\omega_j) = \sum_{n=1}^{2N} y_n(\omega_j) \Gamma_n, \quad (6)$$

where functions $y_n(\omega)$ are known, e.g. for free boundaries see Ref. [9]. If x is the “ordering” direction in a sense that the Pauli matrix σ_n^x [15] measures the spin at site n , then

$$\Gamma_{2n-1} = P_{n-1} \sigma_n^x \quad \Gamma_{2n} = P_{n-1} \sigma_n^y \quad (7)$$

where $P_0 = 1$ and $P_n = \prod_{j=1}^n (-\sigma_j^z)$, $j = 1, \dots, N$ and σ_n^i are Pauli operators [15]. In the customary language, P_n is a string of disordering operators because $(-\sigma_j^z)$ reverses the spin at site j . We emphasise that this method does not give the $X(\omega_j)$ vacuum $|\Phi\rangle$ (the maximal eigenvector, since $\gamma(\omega) \geq 0$) *constructively*, unlike the SML case [15]. The maximum eigenvalue of V is $\Lambda_{max}(N) = \exp(1/2) \sum_{j=1}^N \gamma(\omega_j(N))$ and the free energy $f(N)$ per unit length in the $(1, 0)$ direction is now

$$f(N) = -\frac{1}{2} \sum_{j=1}^N \gamma(\omega_j(N)), \quad (8)$$

valid for $h_1 h_2 \geq 0$. This is evidently quite unlike (3) in form. The function $\gamma(\omega)$ is as $\hat{\gamma}(\omega)$ in (4), but with K_1 and K_2 interchanged. The $\omega_j(N)$, $j = 1, \dots, N$ are the solutions of the discretisation equation imposed by the strip geometry

$$\exp 2iN\omega = \exp i(\delta_1(\omega) + \delta_2(\omega)). \quad (9)$$

In this approach, the interpretation of the angles δ_1 and δ_2 is clear; they are phase shifts for reflection of lattice fermions from the surfaces and (8) is a consistency condition required by the presence of two such bounding surfaces at a *finite* separation N [9, 18]. The functions $\delta(\omega)$, $\delta_j(\omega)$, $j = 1, 2$ are given by the same expressions as $\hat{\delta}(\omega)$, $\hat{\delta}_j(\omega)$, $j = 1, 2$, but with K_1 and K_2 interchanged.

With free boundary, a study of the solutions of (8) and of the non-triviality of the eigenvectors which relate to them mandates that we take the solutions in $(0, \pi)$. In fact, there is one solution in each interval $[\pi(j-1)/N, \pi j/N]$, $j = 1, \dots, N$ provided $K_1^* > K_2$, ($T > T_c$). But for $K_1^* < K_2$, ($T < T_c$), there is a solution as above with $j = 2, \dots, N$. If $j = 1$, there is such a solution but only if $N < (\delta^*)'(0)$. If we take the pair $-\omega_1(N), \omega_1(N)$, then as we pass from $N < (\delta^*)'(0)$ to $N > (\delta^*)'(0)$, there is a *bifurcation* to a pair of imaginary solutions $\omega = \pm iv(N)$, one of which is to be taken in the solution set. For $v(N) > 0$, up to order $\exp(-4N\gamma(0))$ we have

$$v(N) \simeq \hat{\gamma}(0) - 2(\sinh 2K_2 \sinh 2K_1)^{-1} \sinh \hat{\gamma}(0) e^{-2N\hat{\gamma}(0)}, \quad (10)$$

with $\hat{\gamma}(0) = 2(K_1 - K_2^*)$ (see Eq. (4)). The corresponding $\gamma(iv(N))$ is given up to order $\exp(-2N\gamma(0))$

$$\gamma(iv(N)) \simeq 2 \sinh 2K_1^* \sinh \hat{\gamma}(0) e^{-N\hat{\gamma}(0)}, \quad (11)$$

which clearly demonstrates asymptotic degeneracy as $N \rightarrow \infty$ [9–11]. The bifurcation of a solution corresponding to $j = 1$ is a mathematical manifestation of the shift of a pseudocritical temperature in a film with respect to the bulk critical temperature T_c . Recall that in a confined two-dimensional Ising system there is no true ordering phase transition; it becomes exponentially rounded and shifted towards lower temperatures. Such a shift, which is $\sim (1/N)$, has been predicted from a scaling analysis by Nakanishi and Fisher [22].

In order to extract the Casimir free energy from (6), we use a contour integral method with a suitable summation kernel. The first use of a summation kernel in problems of this type, somewhat tangentially, is in Onsager’s calculation of surface tension [21]. There, the wavenumbers are equally spaced. Further, there are applications in stochastic processes [23], and, moreover, the general problem was considered in [9], but in a different context. The contour integral is

$$\frac{1}{2} \sum_{j=1}^N \gamma(\omega_j(N)) = \frac{1}{8\pi i} \oint_C d\omega \gamma(\omega) \frac{1}{F_N(\omega)} \frac{dF_N}{d\omega} + R \quad (12)$$

where $R = -(1/2)(\gamma(0) + \gamma(\pi))$, with summation kernel $F_N(\omega) = e^{2iN\omega} - e^{i(\delta(\omega))}$; the integration contour C surrounds every zero of $F_N(\omega)$ in the strip $-\pi < Re\omega < \pi$, with special attention to the behavior at $\omega = \pm\pi$ and $\omega = 0$. None of these is an allowed value, since the associated eigenfunction is trivial. The terms $\gamma(0)$ and $\gamma(\pi)$ do not report in the thermal Casimir force as they are N -independent. The development of the integral in (12) will be given elsewhere. After extracting the bulk term, we find that the rather different representation are indeed the same. Since (5) has a scaling limit (by direct construction), so does the Casimir free energy in the equivalent form

$$f_{Cas}(N) = -\frac{1}{2} \sum_{j=1}^N \gamma(\omega_j(N)) + \frac{N}{4\pi} \int_{-\pi}^{\pi} \gamma(\omega) d\omega \quad (13)$$

a result which would be difficult to extract from a direct assault on (5). We wish to assess the contribution of a single term in the sum to (13). Provided this has a scaling limit, then it is meaningful to compare it with (5).

In particular, it is pertinent to compare the contribution of $(1/2)\gamma(iv(N))$ coming from a complex mode to the Casimir force in the scaling limit as calculated numerically from (5) (see Eq. (3) in Ref. [17]). This is shown in Fig. 2 for $K_1 = K_2$ and free boundaries. The Casimir force is the negative of derivative of the Casimir free energy with respect to N . Taking the scaling limit as $N \rightarrow \infty$, $\hat{\gamma}(0) \rightarrow 0$,

such that $x = N\hat{\gamma}(0)\text{sgn}(T - T_c)$ is fixed of the contribution to the Casimir force from the imaginary mode, one obtains

$$\mathcal{F}_{Cas}^c = -\frac{\sinh 2K_1^*(T_c)}{2} \frac{1}{N^2} \frac{z^2 \sqrt{x^2 - z^2}}{(|x| + x^2 - z^2)}, \quad (14)$$

for $x < 0$. The function $z(x)$ is calculated from

$$\exp(-2z) = (x + z)/(x - z). \quad (15)$$

For $x < -1$ there is one solution, for which the denominator of (14) is strictly positive. For $-1 < x < 0$ (and incidently for $x > 0$) (15) has no real solution. As one can see from Fig. 2 the imaginary wave number yields the dominant contribution to the scaling function $\Theta(x)$ of the critical Casimir force which is negative. Moreover, its magnitude is larger than that of Θ . From Fig. 2, one can see that the surface state contribution governs the leading decay of the critical Casimir interaction; it can be shown that (14) as $x \rightarrow -\infty$ is $-(1/N^2)(\sinh 2K_1^*(T_c))^{-1}x^2e^{-x}$. At the bifurcation point $x = -1$, $(1/2)\gamma(\omega_1)$ goes to zero and is continuous in its argument. The contribution coming from the real mode ω_1 is large and positive for $-1 < x < 0$ (see blue dashed curve in the inset in Fig. 2) and has to be compensated in order to render the negative critical Casimir force in this interval. This contribution is given by (14) with z replaced by iz , when now z is given by a solution of $\tan(z) = z/x$ for $-1 < x < 1$. The Casimir force for $(++)$ BCs may be obtained from the case of the free BCs by applying duality [16]. In this case there is an asymptotic degeneracy associated with a surface mode *in the $T > T_c$ sector*. Eqs. (14) and (15) can be generalized to the case with the surface fields with h_1 and h_2 such that $h_1h_2 > 0$ [24]. This is an interesting matter because surface fields maybe adjusted to produce both attractive and repulsive Casimir forces. Equally, considering the case $h_1h_2 < 0$ and scaling around the wetting transition but not the bulk critical point, we can produced novel behavior. These are rather detail calculations and results which seemed to the authors to make separate publication advisable.

We now give a more intuitive account of the asymptotic degeneracy. For N large enough, but finite, we will have states in the strip which are either largely positively or largely negatively magnetized. At the transfer matrix level, called these states $|\oplus\rangle$ and $|\ominus\rangle$. We can choose the phases so that the parity operator $P_N |\oplus\rangle = |\ominus\rangle$ (The operator P_N is given by Eq. (7) with $n = N$; note that $P_N^2 = 1$. It is called the parity operator because it reverses all x -quantised spins in the column simultaneously; it is an invariant of the Hamiltonian.) Then the fact that $P_N |\Phi\rangle = |\Phi\rangle$ implies that $|\Phi\rangle = (|\oplus\rangle + |\ominus\rangle)/\sqrt{2}$ and

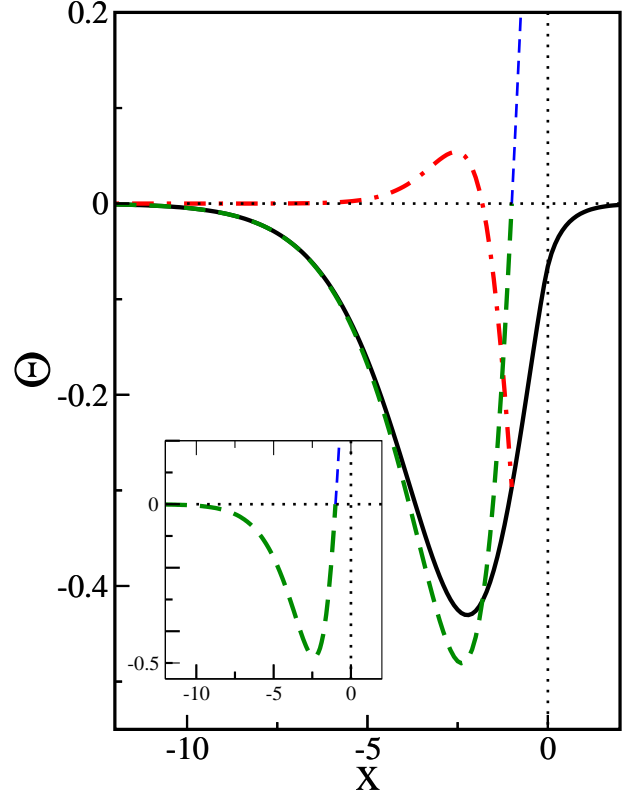


Fig. 2: (color online) The surface mode contribution to the scaling function of the critical Casimir force $\Theta^c = N^2 \mathcal{F}_{Cas}^{(c)}$ for the isotropic ($K_1 = K_2$) Ising strip with free boundary conditions (dashed green line) shown together with the total scaling function $\Theta(x)$ (solid black line). The red dot-dash line is the result of the subtraction of the part coming from the imaginary wave number $k = iv(N)$ from the $\Theta(x)$. The surface mode contribution (the dashed green line) is equal to 0 at $x = -1$. The dashed blue line shows the contribution to the scaling function of the critical Casimir force coming from the real wave number ω_1 for $-1 < x < 0$.

further that $X^\dagger(iv(N)) |\Phi\rangle = (|\oplus\rangle - |\ominus\rangle)/\sqrt{2}$, since $P_N X^\dagger(iv(N)) |\Phi\rangle = -|\Phi\rangle$. It follows that

$$|\oplus\rangle = \frac{(1 + X^\dagger(iv)) |\Phi\rangle}{\sqrt{2}} \quad |\ominus\rangle = \frac{(1 - X^\dagger(iv)) |\Phi\rangle}{\sqrt{2}} \quad (16)$$

The Euclidean “evolution” of these states is instructive: consider the matrix elements $\langle \oplus | V^n | \oplus \rangle = (1 + e^{-n\gamma(iv(N))})/2$ and $\langle \ominus | V^n | \oplus \rangle = (1 - e^{-n\gamma(iv(N))})/2$. Now $\gamma(iv(N)) \sim \hat{\gamma}(0) \exp(-N\hat{\gamma}(0))$ and if $n\hat{\gamma}(0) \gg \exp(N\hat{\gamma}(0))$, the transition matrix element tends to $1/2$, that is, the system dephases on this length scale. Thus the dominant configurations correspond to successive positively and negatively magnetized regions separated by domain walls running across the strip as in the Fisher Privman theory (see Fig. 1c in Ref. [12]). On the other hand, if $n = 1$, then $\langle \ominus | V^n | \oplus \rangle \sim \gamma(iv)/2$ so that magnetic domain reversal is improbable but strictly not impossible if $N < \infty$. Since $\langle \oplus | V^n | \oplus \rangle = \langle \ominus | V^n | \ominus \rangle$, we see

that the wall interactions of the \oplus and \ominus phases are the same, an intuitively obvious result of symmetry. This is the physical reason for the smallness of $\gamma(iv(N))$ in (11). In (6), with $\omega_1 = iv(N)$ we have $y_{2n-1} \sim N_0 \exp(-nv(N))$ and $y_{2n} \sim iN_0 \exp(-(N-n)v(N))$ with $v(N) \simeq \hat{\gamma}(0)$ (N_0 is a suitable normalization constant). The imaginary mode qualifies as a surface state because of the exponential attenuation away from the surface. This is because $\hat{\gamma}(0) > 0$, except at the critical point, which has a new attribute: it is also a de-pinning point for the surface state, simultaneously at both edges as $\hat{\gamma}(0) \rightarrow 0$. In the scaling regime, the two exponentially decaying tails overlap, a physical reason to expect a significant contribution to the Casimir force. The bubble/domain wall, or interface Hamiltonian, idea has proved extremely useful in understanding planar uniaxial models [25–27]. It, too, needs amplification to work with free boundaries: for modes with real $\omega_j(N)$, path fluctuations are controlled by surface stiffness and by repulsion from the edges, as expected. For imaginary mode we have a random succession of domain walls which cross the strip, pointing on average in the $(0, 1)$ direction following Fisher-Privman. Within a stripe with positive magnetization, the state in a column is $|\oplus\rangle$ and it is essentially proved that the expectation value $\langle \oplus | \Gamma_{2n-1} | \oplus \rangle = y_{2n-1}$. Now Γ_{2n-1} consists of a string of disorder operators (the so-called the Jordan-Wigner tail see (7)), thus it creates a column of misfit bonds with which a path may be associated. This path connects the end of the tail at the site n to any point on the boundary. Thus $y_{2n-1} \sim \exp(-n\tau(0, 1))$ where $\tau(0, 1) = \hat{\gamma}(0) = v(N)$ is the surface tension in the $(0, 1)$ direction.

In summary, in this Letter we have obtained the following new results: (1.) Strong asymmetry of the Casimir force, as shown in Fig. 2, is related to the appearance in the spectrum of the transfer matrix of bound states, which are also surface states. (2.) Surface states produce the asymptotic degeneracy of the transfer matrix advocated as a diagnostic for phase transition by Kac [10]. They also play a key role in the realization of Fisher-Privman theory in these systems. The critical point has an additional, new characterisation as an unbinding transition. We interpret the bound state at a microscopic level as a linear combination of block spin reversal operators. (3.) Our results require a significant modification of the interface Hamiltonian concept for these systems.

Occurrence of surface states depends on the boundary conditions of the strip. In a strip with free boundaries the asymptotic degeneracy occurs because the coexistence of two pseudophases in a finite system remains at the same line in the thermodynamic space (vanishing bulk field $h = 0$) as in the bulk system. Surface states form because free boundaries effectively attract domain walls due to the missing neighbours effect. This is analogous to the case of surfaces with wetting boundary conditions below T_c , where the effective attraction due to the missing neighbours is amplified by the action of the surface fields. As a result, the thin film can be formed near the surface

which then undergoes unbinding at the wetting transition. This argument carries over to three dimensional systems. For $(+, +)$ boundary conditions an imaginary wavenumber and the associated asymptotic degeneracy occurs above T_c ; there is no asymptotic degeneracy below T_c because the surface breaks the symmetry and pseudo coexistence is shifted away from the $h = 0$ line. For this boundary conditions, the imaginary mode gives rise to the critical adsorption which is characterized by the magnetization profile which is enhanced near both surfaces and decays to zero in the middle of the strip.

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